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LETTER TO THE EDITOR

Localization in a dynamically disordered, dissipative medium: a model for $1/f$ noise

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Abstract. We study the motion of a quantum particle in a dynamically disordered tight-binding lattice, including a frictional dissipative interaction. The mean square displacement evolves from free-particle motion at initial times approaching a finite stationary form at long times. This localization due to frictional slowing down of diffusion leads to $1/f$ noise, using a scaling argument.

The study of the motion of a quantum particle in a dynamically disordered lattice has attracted much attention recently because of its relevance to various charge and excitation transport processes in molecular solids and, also, to the diffusion of light atoms on solid surfaces.

Here we focus on the simplest case of a one-dimensional tight-binding lattice with dynamically fluctuating energies of one-orbital atomic sites. The long-time motion of a particle, placed initially on a given site of such a lattice, is known to be diffusive [1, 2]. The existence of this diffusive motion has also been confirmed for a quantum particle in a dynamically disordered continuous-space potential [3]. The diffusion constant has, furthermore, been calculated in more general cases, e.g., when both the site energies and the nearest-neighbour hopping integrals have randomly fluctuating components [1] and for higher-dimensional modes [4].

As is well known, the fluctuations of the site energies, which act as a time-dependent random potential, are caused by incoherent thermal vibrations of the lattice. On the other hand, the thermal fluctuations are also affected by the motion of the particle itself and this leads to an additional dissipative frictional force which tends to restore the particle to equilibrium, in much the same way as in Brownian motion theory [5]. The frictional force is expected to play an important role, just as in Brownian motion where its omission changes the motion from diffusive to superdiffusive [6].

In this letter we report a simple analysis of the effect of dissipation on the motion of a quantum particle in a dynamically disordered lattice. As an important by-product, our results suggest a new general explanation for $1/f$ noise in terms of dynamic randomness on a lattice and the concomitant friction.

The correct quantum-mechanical description of dissipation involves the frictional coupling of the particle to a bath of harmonic oscillator degrees of freedom [7].

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However, since this approach is not easy to implement in analytical treatments we shall adopt an alternative description in terms of a simple frictional Hamiltonian [8]

$$H = (p^2/2m)e^{-\gamma t} + V(x,t)e^{\gamma t} \tag{1}$$

which yields a classical Langevin equation of motion with a frictional force $-\gamma p$ and a dynamically fluctuating random force $-\partial V(x,t)/\partial x$. Here $V(x,t)$ is usually taken to be Gaussian and δ-correlated in time:

$$\langle V(x,t)V(x',t')\rangle = V_0^2 g(x-x')\delta(t-t') \tag{2}$$

and $\langle \ldots \rangle$ denotes a statistical average over the ensemble of realizations of $V(x,t)$. Despite some well-known difficulties inherent to the quantization of the Hamiltonian (1), it has been used extensively (for non-random potentials) for describing frictional effects in other systems, e.g. nuclear reactions [8]. In the context of dynamical disorder, the use of random frictional Hamiltonians is supported by a recent quantum-mechanical derivation of Brownian motion based on such a Hamiltonian [9]; since this treatment yields the same mean square displacement at long times as the Langevin model [9], it is believed that the deficiency of (1) from the quantum point of view is unimportant as far as the form of the MSD for $t \to \infty$ is concerned.

In order to describe the analogous frictional dissipation for a lattice we start from the continuum limit (lattice parameter $a \to 0$) of the tight-binding model referred to above, where the Hamiltonian has the form [10]

$$H = -\hbar^2(2m)^{-1}\partial^2/\partial x^2 + V(x,t), V(x,t) = \epsilon(x,t) + 2V.$$

Here $\epsilon(x,t) \equiv \epsilon_j(t)$ is the continuum limit of an electron's site energy in a fixed atomic orbital $|\phi\rangle \equiv |j\rangle$ centred at a site $x = ja$, V is the constant hopping integral between nearest neighbours on the lattice and $m = -\hbar^2(2a^2V)^{-1}$ is the electron's effective mass. After including friction in this continuum Hamiltonian, using the prescription of (1), we revert back to the case of a lattice and obtain the following frictional tight-binding Hamiltonian† [11]:

$$H = \sum_n [\epsilon_n(t)e^{\gamma t} + 4V\sinh\gamma t]|n\rangle\langle n| + Ve^{-\gamma t}\sum_{n,\delta}|n\rangle\langle n+\delta| \qquad \delta = \pm 1 \tag{3}$$

where the dynamically fluctuating site energies $\epsilon_n(t)$ are assumed to have a Gaussian white-noise spectrum

$$\langle \epsilon_m(t)\epsilon_n(t')\rangle = \epsilon_0^2\delta_{m,n}\delta(t-t') \qquad \langle \epsilon_n\rangle = 0. \tag{4}$$

In the continuum limit they correspond to potential fluctuations with a vanishing correlation length, i.e., $g(x-x') = \delta(x-x')$. The tight-binding Hamiltonian (3) with $\gamma = 0$, and fluctuating site energies obeying (4) has been used, in particular, for modelling the motion of carriers in narrow-band molecular solids at high temperatures (see [1, 2] and references therein). As mentioned above, random fluctuations in time of the potential (site energy) are only one part of the effect of the coupling to thermal lattice vibrations—the latter also cause dissipation in the system, as is evident from the fluctuation-dissipation theorem. A consistent treatment of the coupling to

† The Hamiltonian (3) differs from the approximate frictional Hamiltonian for a lattice in the one-band tight-binding limit derived by N Kumar (see [11]).

thermal vibrations must, therefore, include both effects simultaneously. The form of the dependence of the Hamiltonian (1) on the friction constant has been obtained by requiring Hamilton's equations to reduce to the Langevin equation in the classical case. However, due to the lack of a detailed quantum derivation of (1) from the coupling to an oscillator bath describing phonons, it remains essentially phenomenological (for the large body of relevant references and the sense in which (1) is justified quantum mechanically, see the review by Dekker [8]).

In order to study the motion of an electron, we expand the time-dependent wavefunction in the site representation, $\psi(t)\sum_m a_m(t)|m\rangle$, and rewrite Schrödinger's evolution equation for the Hamiltonian (3), $i\hbar\,\partial\psi(t)/\partial t = H\psi(t)$, in the form of coupled equations for the density matrix elements $\rho_{mn}(t) = a_m^*(t)a_n(t)$:

$$i\hbar\frac{d\rho_{mn}}{dt} = e^{\gamma t}[\epsilon_n(t) - \epsilon_m(t)]\rho_{mn} - Ve^{-\gamma t}\sum_\delta(\rho_{m+\delta,n} - \rho_{m,n+\delta}). \tag{5}$$

Since $\rho_{ij}(t)$ are functionals of the set of Gaussian variables $\{\ldots,\epsilon_m(t),\ldots\}$ we can use Novikov's theorem in conjunction with causality (i.e. we assume that $\rho_{ij}(t)$ depends on $\{\ldots\epsilon_m(t')\ldots\}$ for $t' \leqslant t$ only) to derive closed equations for the averages $\langle\rho_{ij}\rangle$, following, essentially, the previous treatments for $\gamma = 0$ [1, 2]. We thus obtain the equations of motion

$$\frac{d\langle\rho_{mn}\rangle}{dt} = -\frac{\epsilon_0^2}{\hbar^2}e^{2\gamma t}(1-\delta_{m,n})\langle\rho_{mn}\rangle + \frac{iV}{\hbar}e^{-\gamma t}\sum_\delta(\langle\rho_{m+\delta,n}\rangle - \langle\rho_{m,n+\delta}\rangle) \tag{6}$$

which will be solved subject to the initial condition $\langle\rho_{mn}(0)\rangle = \rho_{mn}(0) = \delta_{m,0}\delta_{n,0}$ corresponding to a particle located at the origin at $t = 0$. To this end we define Fourier transforms on a lattice with N sites, $a_m(t) = (\sqrt{N})^{-1}\sum_k a_k(t)\exp(ikma)$, using periodic boundary conditions, i.e., $a_{m+N}(t) = a_m(t)$, which yields $k = (2\pi p/Na)$, $p = 0, 1, \ldots, N-1$. Thus by inverting (6) we get

$$\frac{d\rho_{kk'}}{dt} = -\frac{\epsilon_0^2}{\hbar^2}e^{2\gamma t}(\rho_{kk'} - \Lambda_{kk'}) + \frac{2iV}{\hbar}e^{-\gamma t}(\cos ka - \cos k'a)\rho_{kk'} \tag{7}$$

where

$$\rho_{kk'}(t) = N^{-1}\sum_{m,n}\langle\rho_{mn}(t)\rangle\exp(ikma - ik'na) \qquad \rho_{kk'}(0) = N^{-1}$$

and

$$\Lambda_{kk'}(t) = N^{-1}\sum_{k'',k'+k''}\rho_{k+k'',k'+k''}(t).$$

The mean square displacement may be expressed as

$$\langle x^2(t)\rangle = \lim_{N\to\infty}\sum_{j=1}^{N}(ja)^2\langle\rho_{jj}(t)\rangle = -\lim_{N\to\infty,k\to 0}N\mathrm{Re}\frac{\partial^2\Lambda_{k,0}(t)}{\partial k^2}. \tag{8}$$

The equations (7) cannot be solved exactly for $\gamma \neq 0$. However, since we expect $\langle x^2(t)\rangle$ to be proportional to the 'inverse mass' squared (as is, indeed, the case for

$\gamma = 0$), it is sufficient to treat the effect of the hopping term in (7) in second-order perturbation theory. In contrast, the 'potential energy term' must be treated exactly, since, e.g., for $\gamma = 0$, $\langle x^2(t)\rangle$ is proportional to $1/\epsilon_0^2$ [1, 2].

The solution for $\Lambda_{kk'}(t)$, which is exact to order V^2, is given by

$$\Lambda_{kk'}(t) = \frac{1}{N} - \frac{4V^2}{\hbar^2 N}[1 - \cos(k-k')a] \int_0^t t' \, \mathrm{e}^{-\gamma t'} \exp(-\alpha \mathrm{e}^{2\gamma t'}) \int_0^{t'} \mathrm{d}t'' \, \mathrm{e}^{-\gamma t''} \times \left(\frac{\epsilon_0^2}{\hbar^2} \int_0^{t''} \mathrm{d}t''' \, \mathrm{e}^{2\gamma t'''} \exp(\alpha \, \mathrm{e}^{2\gamma t'''}) + \mathrm{e}^{\alpha} \right) \qquad \alpha = \frac{\epsilon_0^2}{2\gamma\hbar^2}. \tag{9}$$

It is obtained by quadratures† from an expansion to successive orders in V of (7) and of the equation

$$\frac{\mathrm{d}\Lambda_{kk'}}{\mathrm{d}t} = \frac{2\mathrm{i}V}{\hbar N} \mathrm{e}^{-\gamma t} \sum_{k''} [\cos(k+k'')a - \cos(k'+k'')a] \rho_{k+k'',k'+k''}$$

which follows from (7), noting that $\Lambda_{k+k'',k'+k''} = \Lambda_{kk'}$ (periodic boundary conditions). From (8) and (9) we then obtain, after some calculations,

$$\langle x^2(t)\rangle = (4V^2a^2/\gamma\hbar^2)[(\epsilon_0^2/\hbar^2) I(\alpha, t) + K(\alpha, t)] \tag{10}$$

where

$$I(\alpha,t) = \int_0^t \mathrm{d}t' \exp -\alpha \mathrm{e}^{2\gamma t'} \int_0^{t'} \mathrm{d}t'' \, \mathrm{e}^{-\gamma(t'-t'')} \exp(\alpha \mathrm{e}^{2\gamma t''})[1 - \mathrm{e}^{-\gamma(t'-t'')}]$$

$$K(\alpha,t) = \mathrm{e}^{\alpha} \int_0^t \mathrm{d}t' \, \mathrm{e}^{-\gamma t'} \exp(\alpha \mathrm{e}^{2\gamma t'})(1 - \mathrm{e}^{-\gamma t'}). \tag{10a}$$

In the limit of weak dissipation, $\gamma \ll \epsilon_0^2/2\hbar^2$, the time integrals may be performed explicitly in the form of a sum of contributions proportional to successive powers of $1/\alpha$. Neglecting exponentially decreasing terms (proportional to $\exp(-\alpha \mathrm{e}^{2\gamma t})$, we obtain, for $\gamma t \gg 1$,

$$\langle x^2(t)\rangle = (2V^2a^2\hbar^2/\epsilon_0^4)[(\epsilon_0^2/2\hbar^2\gamma)(1 - \mathrm{e}^{-4\gamma t}) - 13 - \mathrm{e}^{-6\gamma t} + \mathrm{O}(1/\alpha)]. \tag{11}$$

This shows that the particle remains located within a finite distance $\sqrt{\langle x^2(\infty)\rangle}$ from the initial site, as a result of frictional slowing down of the diffusion [1, 2]. On the other hand, by expanding (10*a*) in powers of γ for $\gamma \to 0$ and retaining zero-order terms, we obtain

$$\langle x^2(t)\rangle = (4V^2a^2/\epsilon_0^2)[t + (\hbar^2/\epsilon_0^2)(\mathrm{e}^{-\epsilon_0^2 t/\hbar^2} - 1)] \tag{12}$$

which is in agreement with the previous results in the absence of dissipation [1, 2].

For the sake of completeness we also include the form of the mean square displacement when the time-dependent random potential vanishes, namely at $T = 0$ (where $\epsilon_0 = 0$ [1, 2]). From (10) and (10*a*) we then have $\langle x^2(t)\rangle = 2V^2a^2\gamma^{-2}\hbar^{-2}(1 - \mathrm{e}^{-\gamma t})^2$, which describes the gradual freezing of the initial ballistic evolution, $\langle x^2(t)\rangle = 2V^2a^2\hbar^{-2}t^2$.

† Also note the identity $N^{-1}\sum[\cos(k+k'')a - \cos(k'+k'')a]^2 = 1 - \cos(k-k')a$.

An important consequence of the constancy of the mean square displacement for $t \to \infty$ is the existence of $1/f$ excess noise [12]. This follows from standard heuristic arguments. The noise associated with a physical variable $x(t)$ is described by the spectral density [13] defined by

$$S(\omega) = 2 \lim_{T\to\infty} \frac{1}{T} \left\langle \left| \int_0^T \mathrm{d}t\, x(t) \mathrm{e}^{\mathrm{i}\omega t} \right|^2 \right\rangle . \tag{13}$$

For a statistically stationary random variable [5], such as the displacement of a particle in the present case ($\langle x^2(t \to \infty)\rangle = \text{constant}$, (11)), this expression simplifies to [5, 13]

$$S(\omega) = 4 \int_0^\infty \mathrm{d}\tau\, \langle x(\tau + t)x(t)\rangle \cos \omega\tau \tag{14}$$

where t is an arbitrary origin within the asymptotic domain of (11). In order to extract the frequency dependence of $S(\omega)$ we then invoke a dynamic scaling assumption similar to that discussed by Marinari *et al* [14]. Thus we assume that for large t the auto correlation function $\langle x(\tau + t)x(t)\rangle$ is determined by the unique length $\xi(t) = \langle x^2(t)\rangle^{1/2}$ such that [15]

$$\langle x(\tau + t)x(t)\rangle = \xi^2(t) f[(\tau + t)/t] \qquad f(1) = 1 \qquad t \to \infty. \tag{15}$$

By inserting this expression in (14), for $t = \omega^{-1}$, $\tau = yt$, we obtain

$$S(\omega) \approx \frac{\xi^2(\omega^{-1})}{\omega} \int_0^\infty \mathrm{d}y\, f(y + 1) \cos y \qquad \omega \to 0 \tag{16}$$

which, according to (11), implies pure low-frequency $1/f$ noise due to the localization of a particle on a lattice under the influence of dynamical randomness and the concomitant dissipation†.

Our model has three very desirable features of a theory of $1/f$ noise:

(i) it yields a pure $1/f$ spectrum at low frequencies, which has proved difficult to achieve theoretically—for example, Marinari *et al* [14] obtain $1/f$ noise only up to a logarithmic correction factor;

(ii) the noise is an equilibrium phenomenon, as is frequently assumed [12, 14]—indeed dynamic correlations of the form (4) with $\epsilon_0^2 \propto T$ are a direct consequence of equilibrium autocorrelations of atomic displacements at temperatures much higher than the Debye phonon energy [1, 2];

(iii) it depends on a general mechanism—a dynamically fluctuating potential (site energies) and the concomitant frictional dissipation—which may be operating in many different systems showing $1/f$ noise at finite temperatures. This mechanism is very similar to the one controlling Brownian motion in the standard Langevin theory.

† The form (16) for $\omega \to 0$ leads to a logarithmic divergence of the LHS of a relation (which follows from (13)) [13] $(2n)^{-1} \int_0^\infty \mathrm{d}\omega\, S(\omega) = \lim_{T\to\infty} T^{-1} \int_0^T \mathrm{d}t\, \langle x^2(t)\rangle$, while the RHS is finite. We note that this drawback is shared by ultra-slow diffusion models of $1/f$ noise such as the Sinai walk on a random medium [14]. In the latter case, using the result for $S(\omega)$ obtained in [14], the LHS of the above relation is found to diverge as $(\ln \omega)^5$ while the RHS diverges as $(\ln t)^4$.

It follows that, just as the Langevin model enables one to understand Brownian motion in different physical systems, the above analysis of a similar model on a lattice may provide a common basis for the $1/f$ noise observed for transport in very diverse systems. The $1/f$ noise is a direct consequence of the localization of the particle in the fluctuating, dissipative medium, which we have demonstrated for the first time. After the submission of this letter we found that the same type of localization and resulting $1/f$ noise also exist for a continuum described by the Hamiltonian (1) with a random potential which is δ-correlated in time as well as in space. This is not surprising, since in the absence of friction the continuum Hamiltonian and the tight-binding Hamiltonian (3) lead to the same type of quantum diffusion [3]. The results for the continuum case have been obtained from a straightforward generalization of the treatment of [3].

We conclude by recalling that we have used the Hamiltonian (3) for the purpose of discussing the effect of the frictional force on the diffusive evolution of the mean square displacement on a lattice at finite temperatures [1, 2]. Since the diffusive motion, which is a basic aspect of our model for dynamic localization, has so far not been derived from a microscopic approach to dynamic disorder [7], a detailed comparison with the latter approach appears premature.

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